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14 OCT 92 14:38:26

U.S. Patent & Trademark Office

P0007

US PAT NO: 3,888,866

L2: 18 of 18

TITLE: Nitrogen derivatives of benzoyl ecgonine

ABSTRACT:
Nitrogen derivatives of benzoyl ecgonine and cocaine are provided, particularly amino, diazonium, and diazo derivatives, the compounds finding use either directly or as intermediates for the preparation of reagents for use in immunoassays. Diazo compounds can be coupled with antigenic materials for the preparation of antibodies to benzoyl ecgonine and/or cocaine. The amino group can be combined with active non-oxo-carbonyl compounds to form reagents which find use in immunoassays.

=> D HIST

(FILE 'USPAT' ENTERED AT 14:31:54 ON 14 OCT 92)
SET PAGELength 62
SET LINELENGTH 78

- L1 78255 S RADIO?
- L2 18 S L1 AND TROPANE#
- L3 1 S L2 AND IODINE
- L4 0 S L2 AND (I-121 OR I-125 OR I-131)
- L5 0 S L2 AND MONOFLUOROALKYL

=> D PNO L2 8,10
8. 4,544,660
10. 4,434,170

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INPUT:

=> file reg

FILE 'REGISTRY' ENTERED AT 12:24:24 ON 14 OCT 92

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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STRUCTURE FILE UPDATES: 10 OCT 92 HIGHEST RN 143899-80-3

DICTIONARY FILE UPDATES: 14 OCT 92 HIGHEST RN 143899-80-3

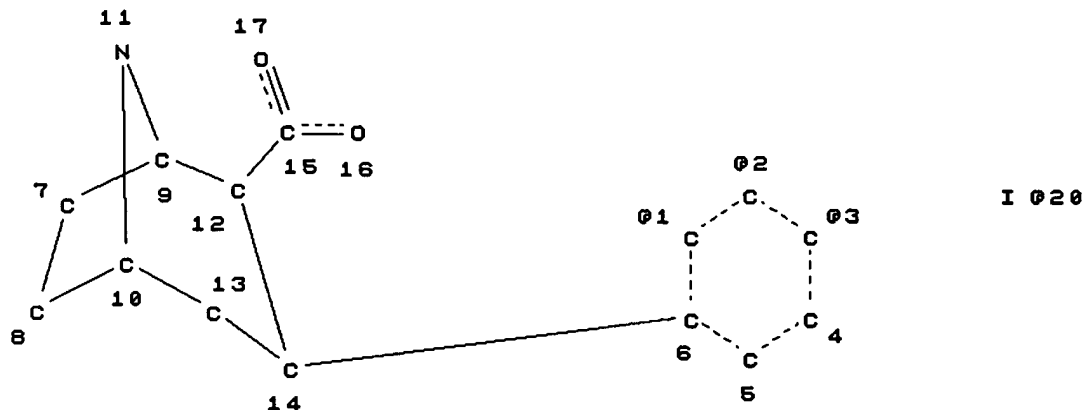
*** YOU HAVE NEW MAIL ***

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=> d que stat 13

L1 STR



VPA 20-1/2/3 U

NODE ATTRIBUTES: NONE

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

L3 17 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 23 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.08

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=> file ca

FILE 'CA' ENTERED AT 12:24:47 ON 14 OCT 92

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FILE COVERS 1967 - 4 Oct 92 (921004/ED) VOL 117 ISS 14.

For OFFLINE Prints or Displays, use the ABS or ALL formats to obtain abstract graphic structures. The AB format DOES NOT display structure diagrams.

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=> d que 16

L1 STR

L3 17 SEA FILE=REGISTRY SSS FUL L1

L4 8 SEA FILE=CA L3

L5 16564 SEA FILE=CA MONOAMINE?/IA

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=> d cbib ab hit 16 1-2

L6 ANSWER 1 OF 2 COPYRIGHT 1992 ACS

CA115(23):251138p Single photon emission computed tomography imaging of monoamine reuptake sites in primate brain with [123I]CIT. Innis, Robert; Baldwin, Ronald; Sybirska, Elzbieta; Zea, Yolanda; Laruelle, Marc; Al-Tikriti, Mohammed; Charney, Dennis; Zoghbi, Sami; Smith, Eileen; et al. (VA Med. Cent., West Haven, CT 06516, USA). Eur. J. Pharmacol., 200(2-3), 369-70 (Eng) 1991. CODEN: EJPHAZ. ISSN: 0014-2999.

AB [123I]CIT [2.beta.-carbomethoxy-3.beta.-(4-iodophenyl)tropane] was evaluated for SPECT (single-photon emission computed tomog.) of dopamine and serotonin reuptake sites in baboon (*Papio anubis*) brain. Highest activities were obsd. in the striatum and reached peak levels at 179 min postinjection. The hypothalamus had the 2nd highest levels, peaking at 45 min after injection. (-)-Cocaine and 2.beta.-carbomethoxy-3.beta.-(4-fluorophenyl)tropane (dopamine and serotonin reuptake inhibitors, resp.) induced rapid and dose-dependent displacement of both striatal and hypothalamic activities. The results indicate that [123I]CIT may be useful for SPECT of dopamine and serotonin reuptake sites in brain.

IT 137433-20-6

(single-photon emission computed tomog. with, of dopamine and serotonin reuptake sites in brain)

L6 ANSWER 2 OF 2 COPYRIGHT 1992 ACS ✓

CA115(21):232566k [123I]-2.beta.-carbomethoxy-3.beta.-(4-iodophenyl)tropane: high-affinity SPECT (single photon emission computed tomography) radiotracer of monoamine reuptake sites in brain. Neumeyer, John L.; Wang, Shaoyin; Milius, Richard A.; Baldwin, Ronald M.; Zea-Ponce, Yolanda; Hoffer, Paul B.; Sybirska, Elzbieta; Al-Tikriti, Mohammed; Charney, Dennis S.; et al. (Res. Biochem. Inc., Natick, MA 01760, USA). J. Med. Chem., 34(10), 3144-6 (Eng) 1991. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CJACS.

AB In order to develop radioligand probes suitable for PET and SPECT imaging of cocaine receptors, iodophenyltropanes I (R = iodo, 123I, R1 = Me; R = iodo, R1 = H) and the 2.alpha. isomer of I (R = iodo R2 = Me) were prepd. from ecgonidine Me ester. I (R = 123I, R1 = Me) was obtained in av. overall yield of 60.0 +/- 13.4% and radiochem. purity of 97.6 +/- 1.6%. The affinities of I (R = iodo, R1 = Me) its epimers, and I (R = F, R1 = Me) for the dopamine and serotonin reuptake sites were detd. from radioligand displacement studies using tissue homogenates prepd. from baboon brain. Highest brain uptake overlay the striatal region and peaked at 154 +/- 19 min post injection and showed striatal to cerebellar ratios of 9.8 +/- 1.6. The in vivo displacement SPECT expts. support the notion that the majority of striatal activity following injection of I (R = 123I, R1 = Me) was assocd. with dopamine reuptake sites.

IT 135416-43-2P

(prepn. and reductive deiiodination of)

IT 136794-86-0P 136794-87-1P 136846-26-9P

(prepn. and uptake of, by brain cocaine receptors)

IT 136846-27-0P 136846-28-1P

(prepn. of)

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=> select hit rn 16 1-2

E1 THROUGH E7 ASSIGNED

=> file reg

FILE 'REGISTRY' ENTERED AT 12:25:36 ON 14 OCT 92

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DICTIONARY FILE UPDATES: 14 OCT 92 HIGHEST RN 143899-80-3

*** YOU HAVE NEW MAIL ***

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1 135416-43-2/RN

1 136794-86-0/RN

1 136794-87-1/RN

1 136846-26-9/RN

1 136846-27-0/RN

1 136846-28-1/RN

1 137433-20-6/RN

L7 7 (135416-43-2/RN OR 136794-86-0/RN OR 136794-87-1/RN OR 136846-26-9/RN OR 136846-27-0/RN OR 136846-28-1/RN OR 137433-20-6/RN)

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=> d ide l7 1-7

L7 ANSWER 1 OF 7 COPYRIGHT 1992 ACS

RN 137433-20-6 REGISTRY

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[4-(iodo-123I)phenyl]-

8-methyl-, methyl ester, (exo,exo)- (9CI) (CA INDEX NAME)

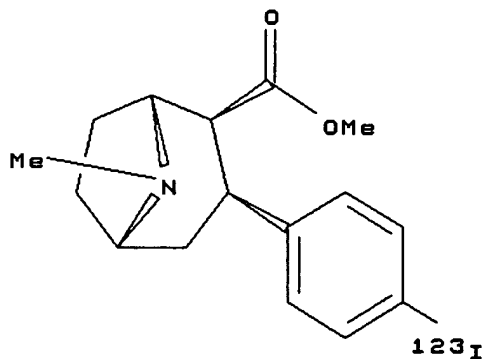
MF C16 H20 I N O2

SR CA

LC CA

DES 2:EXO,EXO

Relative stereochemistry.



2 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 2 OF 7 COPYRIGHT 1992 ACS

RN 136846-28-1 REGISTRY

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, methyl ester, [1R-(2-endo,3-exo)]-, mono(1,5-

naphthalenedisulfonate) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,5-Naphthalenedisulfonic acid, compd. with [1R-(2-endo,3-exo)]-methyl 3-(4-iodophenyl)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid (1:1) (9CI)

MF C16 H20 I N O2 . C10 H8 O6 S2

SR CA

LC CA, CJACS

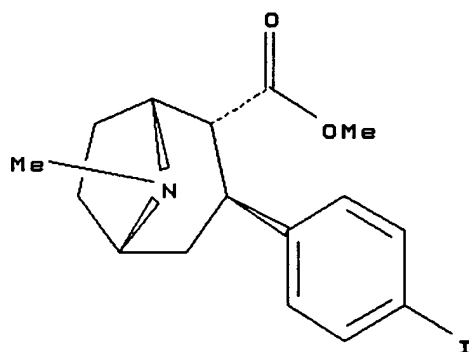
CM 1

CRN 136846-26-9

CMF C16 H20 I N O2

CDES 1:1R2:2-ENDO,3-EXO

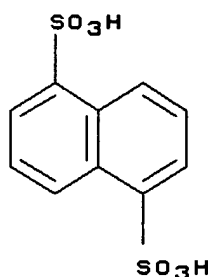
Absolute stereochemistry.



CM 2

CRN 81-04-9

CMF C10 H8 O6 S2



1 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 3 OF 7 COPYRIGHT 1992 ACS

RN 136846-27-0 REGISTRY

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, methyl ester, [1R-(exo,exo)]-, [S-(R*,R*)]-2,3-dihydroxybutanedioate (1:1) (9CI) (CA INDEX NAME)

MF C16 H20 I N O2 . C4 H6 O6

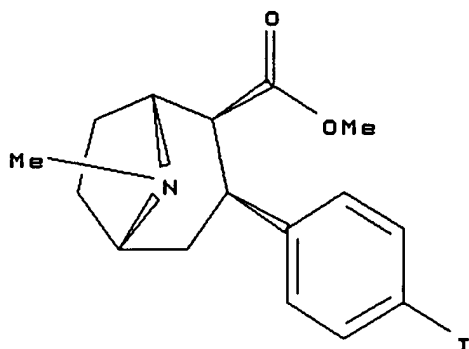
SR CA

LC CA, CJACS

CM 1

CRN 135416-43-2
CMF C16 H20 I N O2
CDES *

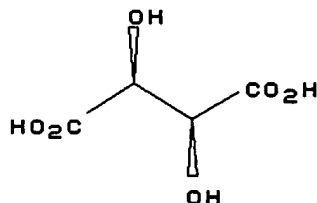
Absolute stereochemistry.



CM 2

CRN 147-71-7
CMF C4 H6 O6
CDES 1:S2:R*,R*

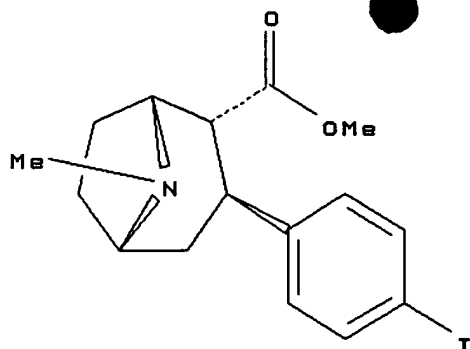
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 4 OF 7 COPYRIGHT 1992 ACS
RN 136846-26-9 REGISTRY
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, methyl ester, [1R-(2-endo,3-exo)]- (9CI) (CA INDEX NAME)
MF C16 H20 I N O2
CI COM
SR CA
LC CA, CJACS
DES 1:1R2:2-ENDO,3-EXO

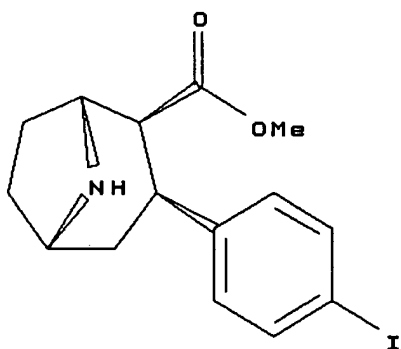
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 5 OF 7 COPYRIGHT 1992 ACS
 RN 136794-87-1 REGISTRY
 CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-, methyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)
 MF C15 H18 I N O2
 SR CA
 LC CA, CJACS
 DES *

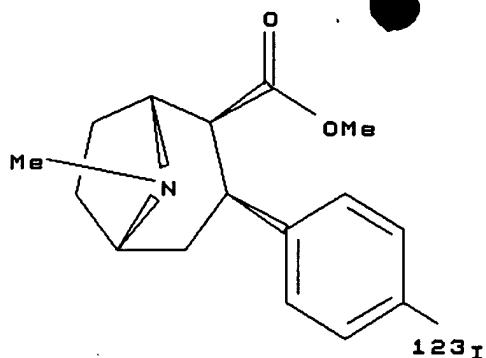
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 6 OF 7 COPYRIGHT 1992 ACS
 RN 136794-86-0 REGISTRY
 CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[4-(iodo-123I)phenyl]-8-methyl-, methyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)
 MF C16 H20 I N O2
 SR CA
 LC CA, CJACS
 DES *

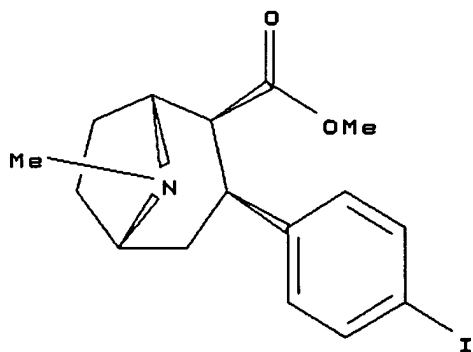
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)

L7 ANSWER 7 OF 7 COPYRIGHT 1992 ACS
 RN 135416-43-2 REGISTRY
 CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, methyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)
 MF C16 H20 I N O2
 CI COM
 SR CA
 LC CA, CJACS
 DES *

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1967 TO DATE)

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